



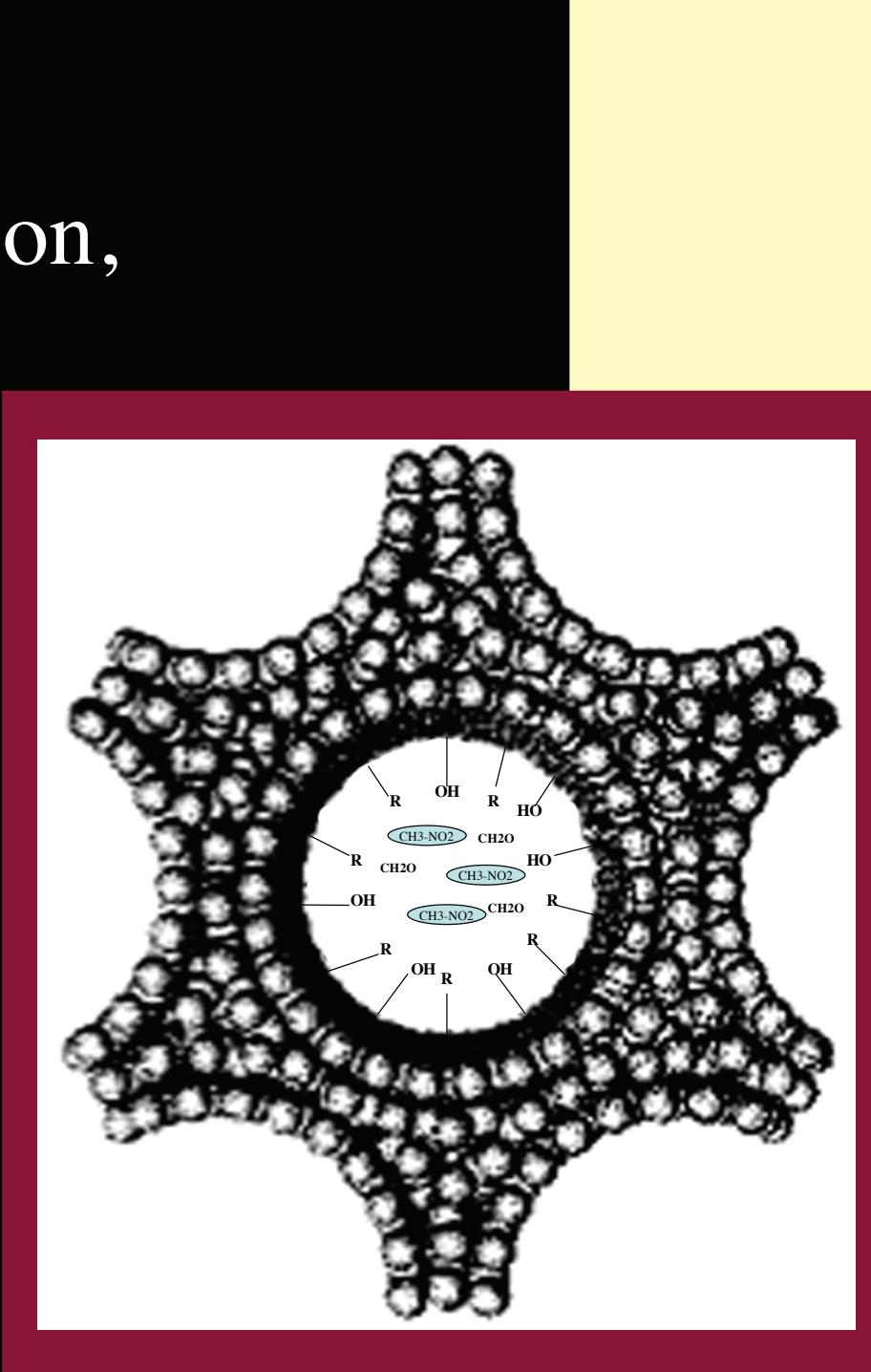
# GAMESS

## General Atomic and Molecular Electronic Structure System

### Parallel Electronic Structure Theory

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Fedorov, Andrey Asadchev,  
Theresa Windus (ISU), Graham Fletcher (Daresbury Laboratory),  
Joseph Ivanic (NCI), Ricky Kendall (ORNL),  
Shiro Koseki (Osaka City University)

- Gradients for Correlated Wavefunctions
- Analytical Vibrational Frequencies
- Parallel CI/MCSCF
- DDRHF, DDMP2
- DDCPHF for analytical hessians
- DDI [1], GDDI
- MRMP2, MCQDPT
- Coupled Cluster, CCSD(T)
- Numerical Derivatives



### New Models for Solvation

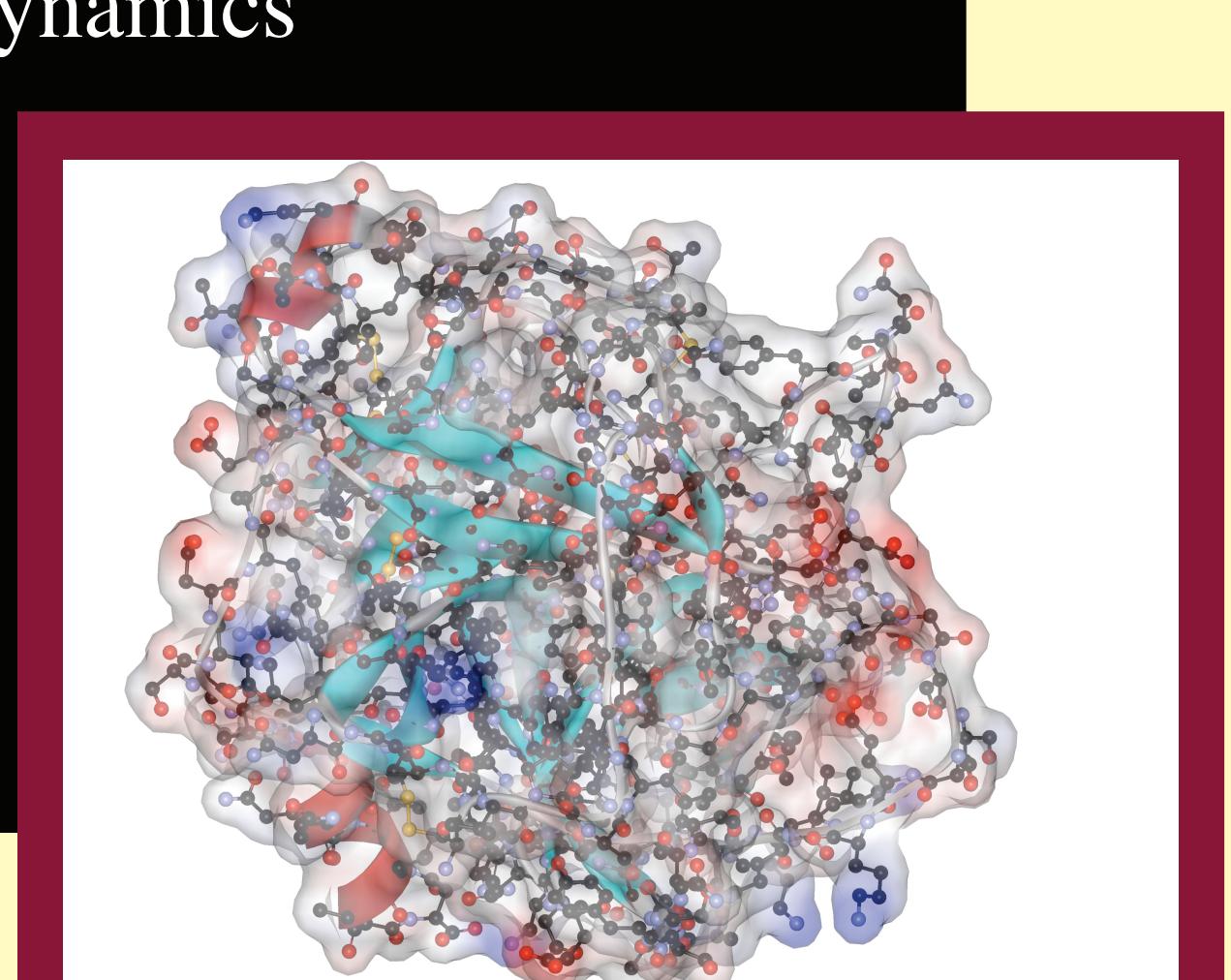
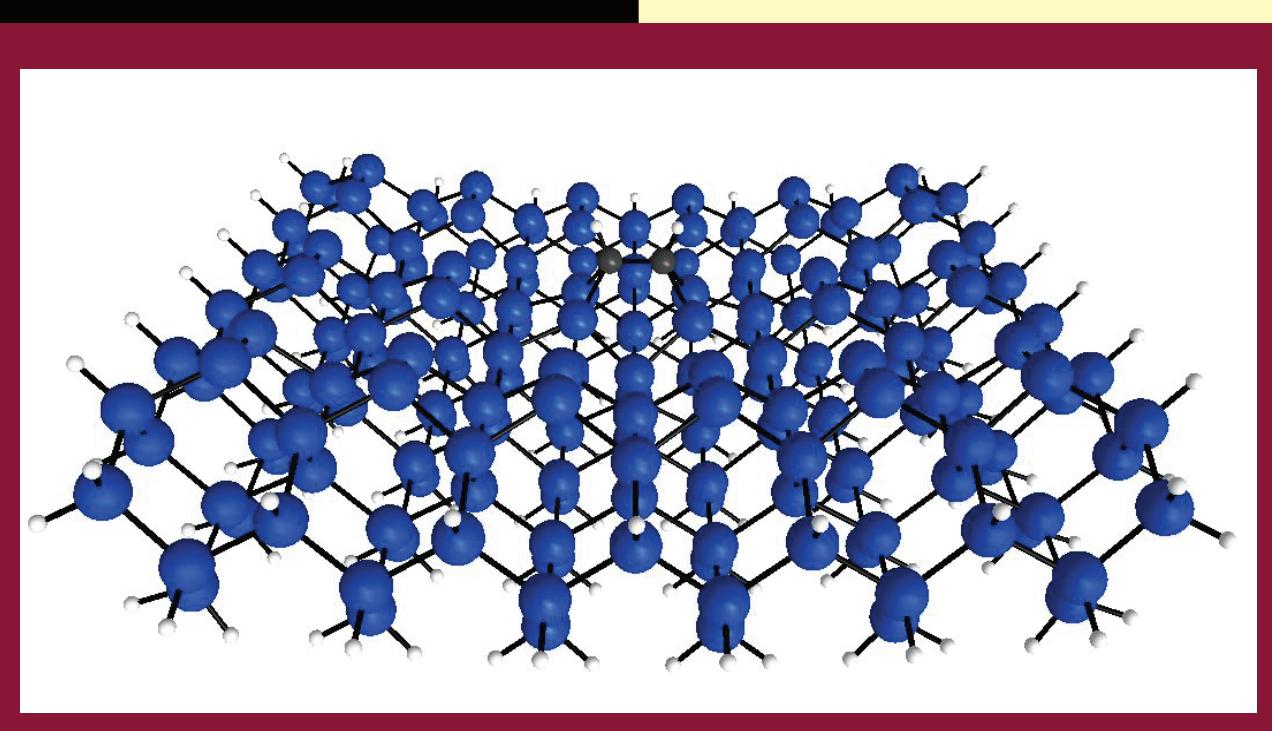
Dan Kemp, Pooja Arora, Federico Zahariev, Spencer  
Pruitt, Hui Li, Ivana Adomovic, Heather Netzloff, Jie  
Song, Grant Merrill, Noriyuki Minezawa, Peng Xu,  
Lyudmila Slipchenko, Tony Smith,  
Jonathan Mullin, SooHaeng Yoo (ISU),  
Simon Webb, Jan Jensen, Vizvaldis Kairys (University of Iowa),  
Paul Day (Wright Laboratories),  
Walter Stevens, Mo Krauss, Dave Garmer (CARB),  
Mark Freitag (Creighton University)

- Solute treated with “correct” ab initio Quantum Mechanics
- Option to include some waters as part of ab initio super molecule
- “First Solvation Shell” treated with effective fragments using model potential derived from accurate Quantum Mechanics [2]
- Structures determined with Monte Carlo and Molecular Dynamics
- Applications: Effect of solvation on reaction thermodynamics, dynamics, photochemistry, π stacking
- Interface with Continuum Models
- Fragment Molecular Orbital Method
- Linear and Nonlinear Response

Summary of current program capabilities:

Run Type	SCF Type				
	RHF	ROHF	UHF	GVB	MCSCF
Energy	CDFP	CDP	CDP	CDP	CDFP
Analytic Gradient	CDFP	CDP	CDP	CDP	CDFP
Numerical Hessian	CDFP	CDP	CDP	CDP	CDP
Analytic Hessian	CDP	CDP	-	CDP	CDP
MP2 Energy	CDFP	CDP	CDP	-	CDP
MP2 Gradient	CDFP	DP	CDP	-	-
CC Energy	CDFP	CD	-	-	-
EOMCC	CD	CD	-	-	-
CI Energy	CDP	CDP	-	CDP	CDP
CIS Gradient	CDP	-	-	-	-
DFT Energy	CDFP	CDP	CDP	-	-
DFT Gradient	CDFP	CDP	CDP	-	-
TDDFT Energy	CD	-	-	-	-
TDDFT Gradient	CD	-	-	-	-
MOPAC Energy	yes	yes	yes	yes	-
MOPAC Gradient	yes	yes	yes	-	-

C= conventional storage of AO integrals on disk  
D= direct evaluation of AO integrals  
F= Fragment Molecular Orbital enabled  
P= parallel execution



### Methods for Potential Energy Surface Crossings and Excited States

Tim Dudley, Dmitri Fedorov, Mike Schmidt, Noriyuki Minezawa, Soohaeng Yoo, Federico Zahariev (ISU), Joseph Ivanic (DOD), Simon Web, Klaus Ruedenberg (Ames Laboratory), Jeff Gour, Piotr Piecuch, Marta Wloch (Michigan State University),  
Jerry Boatz (AFRL-Edwards), Shiro Koseki (Osaka State University)  
-Spin-orbit Coupling, Vibronic Coupling  
-Proton Transfer-Proton treated Quantum Mechanically  
-EOM-Coupled Cluster

### New Methods for Surface Chemistry

Cheol Ho Choi, Jamie Rintelman, Sergey Varganov, Ryan Olson, Yoshinobu Akinaga, Hiroyuki Tamura, Deborah Zorn, Luke Roskop (ISU), Klaus Ruedenberg (Ames Laboratory) Jim Shoemaker, Larry Burggraf (AFIT)  
-SIMMOM Method [3]  
-Linear Scaling Quantum Calculations [4]

### Analysis of Molecular Wavefunctions

Laimus Bytautas, Klaus Ruedenberg (Ames Laboratory), Joseph Ivanic (DOD), Mike Schmidt (ISU)  
- Rigorous “Atoms in Molecules” (AIM) approach  
- Enhanced predictions for the behavior and properties of future materials

### References

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G.D. Fletcher, M.W. Schmidt, M.S. Gordon, Adv. Chem. Physics (invited), 110, 267(1999).  
M.S. Gordon, M. W. Schmidt, Theory and Applications of Comp. Chem., Ch. 41 (2005).
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R.M. Olson, et. al., in: Proceedings of SuperComputing 2003 (IEEE Comp. Soc. Press).
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M.S. Gordon, L. Slipchenko, H. Li, J. H. Jensen, Ann. Rep. Comp. Chem. 3, 177 (2007).
- [3] SIMMOM: C.H. Choi, M.S. Gordon, J. Am. Chem. Soc. 121,11311 (1999).
- [4] Linear Scaling: C.H. Choi, et. al. J. Chem. Phys. 111,8825 (1999).